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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS 3	NOV 26	MARPAT enhanced with FSORT command
NEWS 4	NOV 26	CHEMSAFE now available on STN Easy
NEWS 5	NOV 26	Two new SET commands increase convenience of STN searching
NEWS 6	DEC 01	ChemPort single article sales feature unavailable
NEWS 7	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS 8	DEC 17	Fifty-one pharmaceutical ingredients added to PS
NEWS 9	JAN 06	The retention policy for unread STNmail messages will change in 2009 for STN-Columbus and STN-Tokyo
NEWS 10	JAN 07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent Classification Data
NEWS 11	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 12	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 13	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS 14	FEB 10	COMPENDEX reloaded and enhanced
NEWS 15	FEB 11	WTEXTILES reloaded and enhanced
NEWS 16	FEB 19	New patent-examiner citations in 300,000 CA/CAplus patent records provide insights into related prior art
NEWS 17	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS 18	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS 19	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS 20	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS 21	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS 22	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS 23	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats
NEWS 24	MAR 11	EPFULL backfile enhanced with additional full-text applications and grants
NEWS 25	MAR 11	ESBIOBASE reloaded and enhanced
NEWS 26	MAR 20	CAS databases on STN enhanced with new super role for nanomaterial substances
NEWS 27	MAR 23	CA/CAplus enhanced with more than 250,000 patent equivalents from China

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

```
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:07:59 ON 24 MAR 2009

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.44       0.44

FILE 'REGISTRY' ENTERED AT 11:08:59 ON 24 MAR 2009
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DICTIONARY FILE UPDATES:  22 MAR 2009  HIGHEST RN 1125392-64-4

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.48       0.92

FILE 'REGISTRY' ENTERED AT 11:09:43 ON 24 MAR 2009
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provided by InfoChem.
```

STRUCTURE FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4
DICTIONARY FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

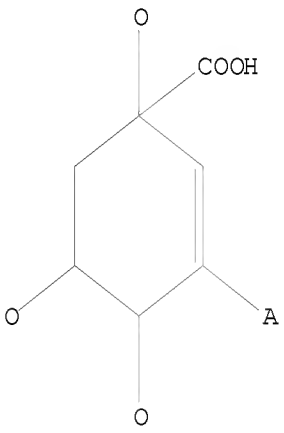
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10565348\10565348 RCE core.str

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR



Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam
SAMPLE SEARCH INITIATED 11:11:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   255 TO ITERATE

100.0% PROCESSED   255 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 4142 TO   6058
PROJECTED ANSWERS: 0 TO   0

L2   0 SEA SSS SAM L1

=> search l1 sss full
FULL SEARCH INITIATED 11:11:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5060 TO ITERATE

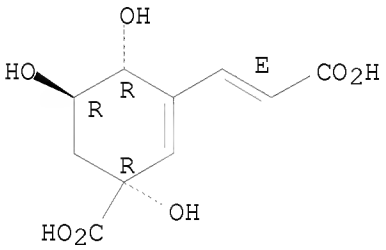
100.0% PROCESSED 5060 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.01

L3 18 SEA SSS FUL L1

=> d scan

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 3-[(1E)-2-carboxyethenyl]-1,4,5-trihydroxy-, (1R,4R,5R)-
MF C10 H12 O7

Absolute stereochemistry.
Double bond geometry as shown.

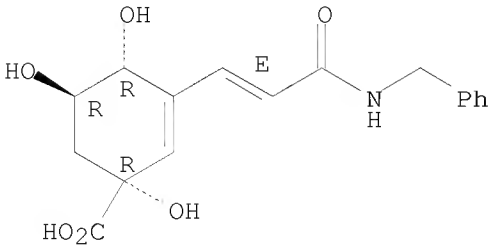


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):18

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-oxo-3-[(phenylmethyl)amino]-1-propen-1-yl]-, (1R,4R,5R)-
MF C17 H19 N O6

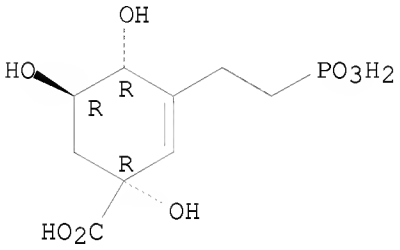
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-(2-phosphonoethyl)-, (1R,4R,5R)-
MF C9 H15 O8 P

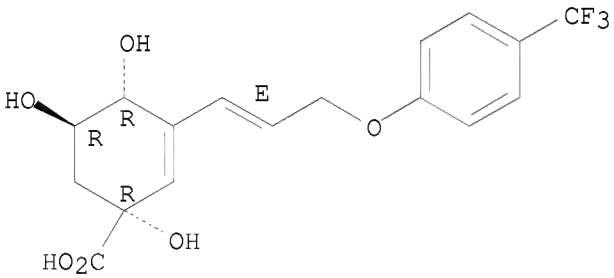
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-[4-(trifluoromethyl)phenoxy]-1-propen-1-yl]-, (1R,4R,5R)-
MF C17 H17 F3 O6

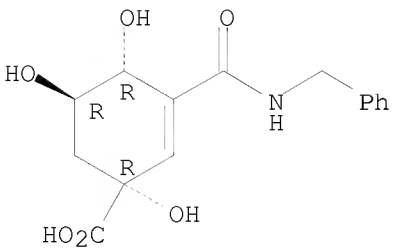
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[(phenylmethyl)amino]carbonyl]-, (1R,4R,5R)-
MF C15 H17 N O6

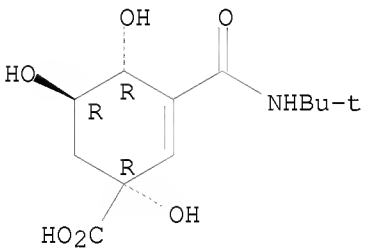
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 3-[[(1,1-dimethylethyl)amino]carbonyl]-1,4,5-trihydroxy-, (1R,4R,5R)-
MF C12 H19 N O6

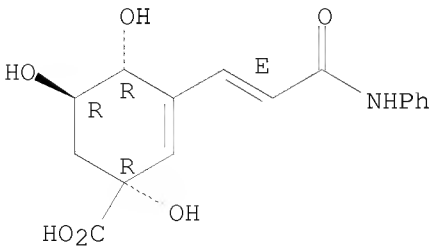
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-oxo-3-(phenylamino)-1-propen-1-yl]-, (1R,4R,5R)-
MF C16 H17 N O6

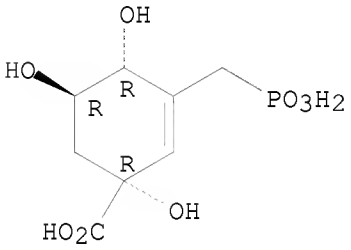
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-(phosphonomethyl)-, (1R,4R,5R)-
MF C8 H13 O8 P

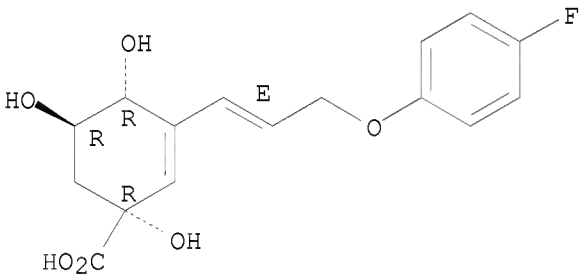
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 3-[(1E)-3-(4-fluorophenoxy)-1-propen-1-yl]-1,4,5-trihydroxy-, (1R,4R,5R)-
MF C16 H17 F O6

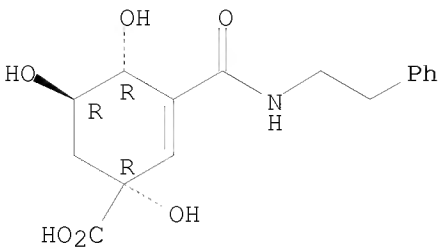
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[(2-phenylethyl)amino]carbonyl]-, (1R,4R,5R)-
MF C16 H19 N O6

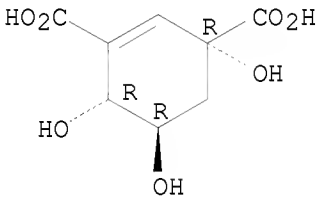
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1-Cyclohexene-1,3-dicarboxylic acid, 3,5,6-trihydroxy-, (3R,5R,6R)-
MF C8 H10 O7

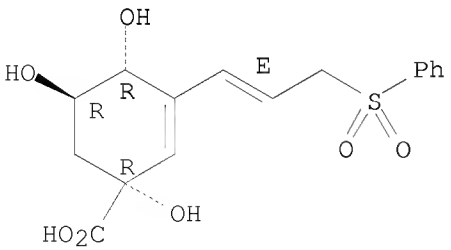
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-(phenylsulfonyl)-1-propen-1-yl]-, (1R,4R,5R)-
MF C16 H18 O7 S

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

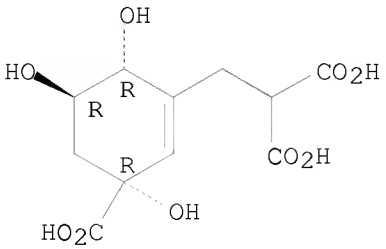


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Propanedioic acid, 2-[[(3R,5R,6R)-3-carboxy-3,5,6-trihydroxy-1-cyclohexen-1-yl]methyl]-
MF C11 H14 O9

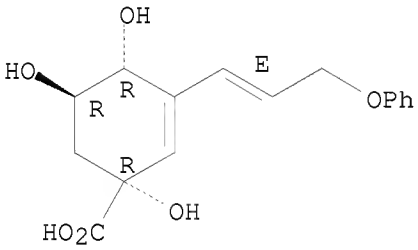
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-phenoxy-1-propen-1-yl]-, (1R,4R,5R)-
MF C16 H18 O6

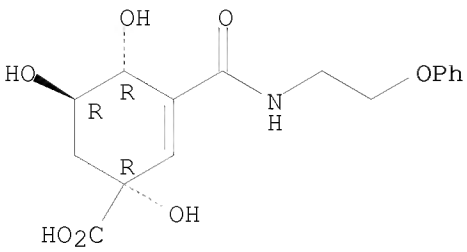
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[[(2-phenoxyethyl)amino]carbonyl]-, (1R,4R,5R)-
MF C16 H19 N O7

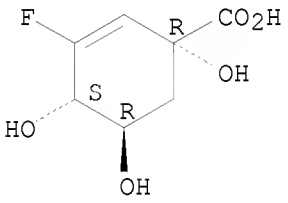
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-
MF C7 H9 F O5

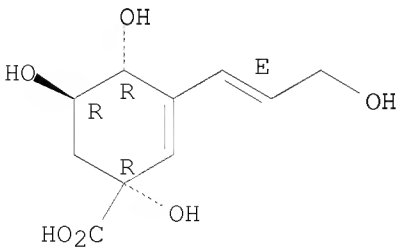
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(1E)-3-hydroxy-1-propen-1-yl]-, (1R,4R,5R)-
MF C10 H14 O6

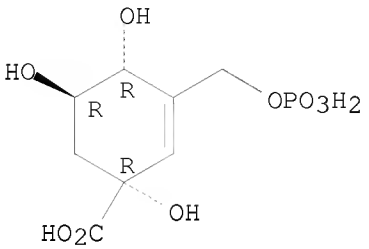
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 18 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 2-Cyclohexene-1-carboxylic acid, 1,4,5-trihydroxy-3-[(phosphonooxy)methyl]-, (1R,4R,5R)-
MF C8 H13 O9 P

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	187.80	188.72

FILE 'CAPLUS' ENTERED AT 11:12:55 ON 24 MAR 2009

FILE COVERS 1907 - 24 Mar 2009 VOL 150 ISS 13
FILE LAST UPDATED: 23 Mar 2009 (20090323/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> l3
L4            6 L3

=> d l4 1-6 ti fbib abs

L4   ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2009 ACS on STN
TI   Rational design, synthesis, and evaluation of nanomolar type II
     dehydroquinase inhibitors
AN   2007:808773  CAPLUS <<LOGINID::20090324>>
DN   147:268289
TI   Rational design, synthesis, and evaluation of nanomolar type II
     dehydroquinase inhibitors
AU   Payne, Richard J.; Peyrot, Fabienne; Kerbarh, Olivier; Abell, Andrew D.;
     Abell, Chris
CS   Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, UK
SO   ChemMedChem (2007), 2(7), 1015-1029
     CODEN: CHEMGX; ISSN: 1860-7179
PB   Wiley-VCH Verlag GmbH & Co. KGaA
DT   Journal
LA   English
OS   CASREACT 147:268289
AB   The in silico design, synthesis, and biol. evaluation of ten potent type
     II dehydroquinase inhibitors are described.  These compds. contain an
     anhydroquinate core, incorporated as a mimic of the enolate reaction
     intermediate.  This substructure is attached by a variety of linking units
     to a terminal Ph group that binds in an adjacent pocket.  Inhibitors were
     synthesized from (-)-quinic acid using palladium-catalyzed Stille and
     carboamidation chemical  Several inhibitors exhibited nanomolar inhibition
     consts. against type II dehydroquinases from Streptomyces coelicolor and
     Mycobacterium tuberculosis.  These are among the most potent inhibitors of
     these enzymes reported to date.
RE.CNT  32    THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4   ANSWER 2 OF 6  CAPLUS  COPYRIGHT 2009 ACS on STN
TI   Nanomolar inhibition of type II dehydroquinase based on the enolate
     reaction mechanism
AN   2007:341043  CAPLUS <<LOGINID::20090324>>
DN   147:671
TI   Nanomolar inhibition of type II dehydroquinase based on the enolate
     reaction mechanism
AU   Toscano, Miguel D.; Payne, Richard J.; Chiba, Akira; Kerbarh, Olivier;
     Abell, Chris
CS   Department of Chemistry, University Chemical Laboratory, University of
     Cambridge, Cambridge, CB2 1EW, UK
SO   ChemMedChem (2007), 2(1), 101-112
     CODEN: CHEMGX; ISSN: 1860-7179
PB   Wiley-VCH Verlag GmbH & Co. KGaA
DT   Journal
LA   English
OS   CASREACT 147:671
GI
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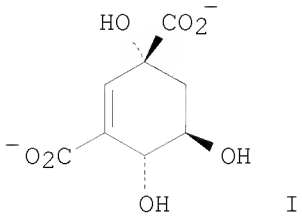

I

AB The authors describe the rational design of a novel, highly potent inhibitor of type II dehydroquinase, the dicarboxylate (I). The incorporation of a carboxylate at the 3-position mimics the putative enolate intermediate in the reaction mechanism, and allows a potential electrostatic binding interaction with the arginine on the active site flap. This results in a 1000-fold increase in potency, making the dicarboxylate I the most potent inhibitor of type II dehydroquinase reported to date, with a high ligand efficiency of -0.68 kcal mol-1 per nonhydrogen atom. The systematic dissection of I in compds. 7-12, all of which show a drop in potency, confirm the synergistic importance of the two carboxylates, the C3 and C4 hydroxyl groups, and the anhydroquinate ring structure for the potency of I.

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
TI Hot off the press
AN 2004:746639 CAPLUS <<LOGINID::20090324>>
DN 142:350581
TI Hot off the press
AU Hill, Robert A.; Sutherland, Andrew
CS Department of Chemistry, Glasgow University, Glasgow, G12 8QQ, UK
SO Natural Product Reports (2004), 21(4), H13-H15
CODEN: NPRRDF; ISSN: 0265-0568
PB Royal Society of Chemistry
DT Journal; General Review
LA English
AB A review covering a selection of 36 recent papers is presented the examines various aspects of current developments in bioorg. chemical and novel natural products such as bielschowskyin which has a novel diterpenoid framework and shows antimalarial and anticancer activity.

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
TI (1R,4S,5R)-3-Fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid: the fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases
AN 2004:422880 CAPLUS <<LOGINID::20090324>>
DN 141:140692
TI (1R,4S,5R)-3-Fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid: the fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases
AU Frederickson, Martyn; Roszak, Aleksander W.; Coggins, John R.; Lapthorn, Adrian J.; Abell, Chris
CS University Chemical Laboratory, Cambridge, CB2 1EW, UK
SO Organic & Biomolecular Chemistry (2004), 2(11), 1592-1596
CODEN: OBCRAK; ISSN: 1477-0520
PB Royal Society of Chemistry
DT Journal
LA English

OS CASREACT 141:140692
AB The fluoro analog of the enolate intermediate in the reaction catalyzed by type II dehydroquinases has been prepared from naturally occurring (-)-quinic acid over seven steps and has been shown to be the most potent inhibitor reported to date of the type II enzyme from Mycobacterium tuberculosis.
RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
TI Vinyl fluoride as an isoelectronic replacement for an enolate anion: Inhibition of type II dehydroquinases
AN 2002:647422 CAPLUS <<LOGINID::20090324>>
DN 138:102740
TI Vinyl fluoride as an isoelectronic replacement for an enolate anion: Inhibition of type II dehydroquinases
AU Frederickson, Martyn; Coggins, John R.; Abell, Chris
CS University Chemical Laboratory, Cambridge, CB2 1EW, UK
SO Chemical Communications (Cambridge, United Kingdom) (2002), (17), 1886-1887
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 138:102740
AB A vinyl fluoride analog of the intermediate in the reaction catalyzed by type II dehydroquinase enzymes has been synthesized over seven steps from (-)-quinic acid and shown to be a potent enzyme inhibitor.
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
TI Cyclohexenyl and Cyclohexylidene Inhibitors of 3-Dehydroquinate Synthase: Active Site Interactions Relevant to Enzyme Mechanism and Inhibitor Design
AN 1997:528717 CAPLUS <<LOGINID::20090324>>
DN 127:216861
OREF 127:42125a,42128a
TI Cyclohexenyl and Cyclohexylidene Inhibitors of 3-Dehydroquinate Synthase: Active Site Interactions Relevant to Enzyme Mechanism and Inhibitor Design
AU Montchamp, Jean-Luc; Frost, J. W.
CS Contribution from the Department of Chemistry, Michigan State University, East Lansing, MI, 48824, USA
SO Journal of the American Chemical Society (1997), 119(33), 7645-7653
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Cyclohexenyl and cyclohexylidene inhibitors possessing strategically placed olefinic residues, in general, bind to 3-dehydroquinate (DHQ) synthase more tightly than similarly substituted cyclohexyl inhibitors. All of the newly synthesized inhibitors were prepared from a common DHQ derivative Cyclohexenyl phosphate 1 is the most potent inhibitor of DHQ synthase thus far identified with an inhibition constant (Ki = 1.2+10-10 M), indicating active site binding 1000-fold tighter relative to the corresponding cyclohexyl phosphate 5. Cyclohexenyl tricarboxylate 2 binds 700-fold more tightly than similarly substituted cyclohexyl tricarboxylate 6 and is the first example of a nanomolar-level inhibitor (Ki = 8.6+10-9 M) possessing neither a phosphate monoester or a phosphonic acid. Cyclohexenyl homophosphonate 4 (Ki = 3.0+10-8 M) and cyclohexylidene homophosphonate 10 (Ki = 3.2+10-9 M) bind 57- and 530-fold, resp., more tightly than the corresponding cyclohexyl

homophosphonate 8. Cyclohexylidene homophosphonate 10 is the first example of a nanomolar-level, homophosphonic acid inhibitor of DHQ synthase. Cyclohexylidene phosphonate 9 (Ki = 2.9+10-10 M) is a 2.9-fold more potent inhibitor relative to cyclohexyl phosphonate 7 which was previously the most potent, slowly-reversible inhibitor of DHQ synthase. Cyclohexenyl phosphonate 3 (Ki = 1.2+10-9 M) is the only olefin-containing, carbocyclic inhibitor where improved binding over the corresponding cyclohexyl analog was not observed The impact of olefinic residues in inhibitors on active site binding may indicate that DHQ synthase plays an active catalytic role during E1cb elimination of inorg. phosphate from enzyme-bound substrate.

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	31.50	220.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.92	-4.92

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SESSION RESUMED IN FILE 'CAPLUS' AT 11:38:19 ON 24 MAR 2009
FILE 'CAPLUS' ENTERED AT 11:38:19 ON 24 MAR 2009
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	31.50	220.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.92	-4.92

=> d l4 5 it

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
IT Enzyme kinetics
(of inhibition; vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT Crystal structure
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
IT 486430-86-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure properties; vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)

IT 486430-83-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)

IT 77-95-2, (-)-Quinic acid 109-87-5 149-73-5 176798-33-7 227002-11-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)

IT 176798-26-8P 183474-88-6P 183475-04-9P 486430-85-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)

IT 486430-84-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)

IT 9012-66-2, E.C. 4.2.1.10
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(vinyl fluoride as an isoelectronic replacement for an enolate anion: inhibition of type II dehydroquinases)

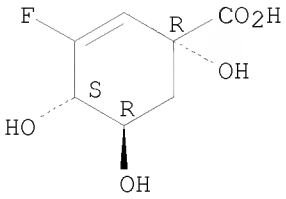
=> 486430-83-5
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L6 3 L5

=> display hitstr l6 1-3

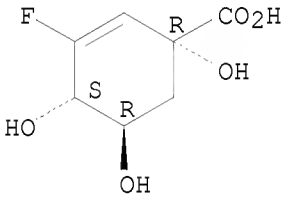
L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
IT 486430-83-5
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(current developments in bioorg. chemical and novel natural products)
RN 486430-83-5 CAPLUS
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-
(CA INDEX NAME)

Absolute stereochemistry.



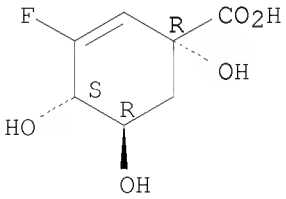
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
IT 486430-83-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)
RN 486430-83-5 CAPLUS
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-(CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
IT 486430-83-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
RN 486430-83-5 CAPLUS
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-(CA INDEX NAME)

Absolute stereochemistry.



=> logoff hold
COST IN U.S. DOLLARS SINCE FILE TOTAL

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FULL ESTIMATED COST	11.16	233.24

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.92

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.16	233.24

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.92

=> d l4 3 it

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
IT Natural products
RL: BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(current developments in bioorg. chemical and novel natural products)
IT 10606-72-1P 128946-78-1P 178948-66-8P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(current developments in bioorg. chemical and novel natural products)
IT 50-99-7, D-Glucose, biological studies 1603-79-8 71155-04-9
72909-34-3, Pyrroloquinoline quinone 108605-69-2, Avenanthramide B
486430-83-5 697299-12-0
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(current developments in bioorg. chemical and novel natural products)
IT 51532-30-0, (S)-4-Methyl-3-heptanone 149008-32-2,
Phomacta-1(14),3,7-triene 689285-37-8, Mikamicranolide 694440-86-3,
Clionastatin A 694440-87-4, Clionastatin B 701203-40-9, Corianlactone
714954-37-7, Psymberin 719296-43-2, Carijenone 719298-06-3,
Bisavenanthramide B 720681-08-3, Stolonilactone 720681-62-9,
Oxaspirosuberitenone 720685-82-5, Sequosempervirin A 742088-25-1,
Gymnorrhizol 790710-32-6, Spirodepressolide
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence)
(current developments in bioorg. chemical and novel natural products)
IT 697298-90-1, Bielschowskysin
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); THU

(Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(current developments in bioorg. chemical and novel natural products)
IT 677025-48-8, Menisporopsin A 681456-07-5 682334-57-2, Brasilienosophyllic acid A 725254-09-1, Abyssomicin C
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(current developments in bioorg. chemical and novel natural products)
IT 339541-50-3, Prerapamycin 360555-98-2, Spongidepsin
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)
(current developments in bioorg. chemical and novel natural products)

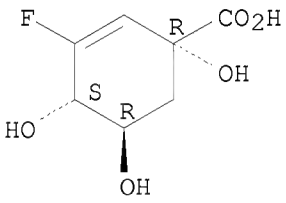
=> 486430-83-5
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L8 3 L7

=> display hitstr l8 1-3

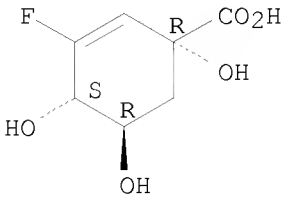
L8 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
IT 486430-83-5
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(current developments in bioorg. chemical and novel natural products)
RN 486430-83-5 CAPLUS
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-
(CA INDEX NAME)

Absolute stereochemistry.



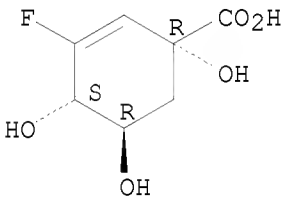
L8 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
IT 486430-83-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)
RN 486430-83-5 CAPLUS
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-
(CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2009 ACS on STN
IT 486430-83-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(vinyl fluoride analog as isoelectronic replacement for an enolate anion and inhibitor of type II dehydroquinases)
RN 486430-83-5 CAPLUS
CN 2-Cyclohexene-1-carboxylic acid, 3-fluoro-1,4,5-trihydroxy-, (1R,4S,5R)-(CA INDEX NAME)

Absolute stereochemistry.



=> d l4 4 it

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
IT Cyclitols
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(fluoro; preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)
IT Mycobacterium tuberculosis
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)
IT 9012-66-2
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)
IT 13019-10-8P 486430-83-5P 486430-84-6P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-

carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 177284-79-6P 725738-25-0P
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 77-95-2, (-)-Quinic acid 177284-85-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 176798-26-8P 183474-88-6P 183475-04-9P 486430-85-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

IT 177284-86-5P 177284-87-6P 486430-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (1R,4S,5R)-3-fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid analogs and their inhibition of bacterial dehydroquinases)

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.54	249.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.92

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